THEORETICAL ASPECTS OF TOPOLOGICALLY UNQUENCHED QCD

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I give an outline of my recent proposal to take the QCD functional determinant in lattice simulations partially into account: The determinant is split into two factors, the factor referring to a standard background in each topological sector is kept exactly, the factor describing the effect of the smooth deviation of the actual configuration from the reference background is replaced by one. The issue of how to choose the reference configurations is discussed and it is argued that "topologically unquenched QCD" is an interesting starting point to study full QCD in lattice simulations as it gets the main qualitative features right from the beginning.

1 What's wrong with quenched QCD ?

In QCD the fermion functional determinant is a nonlocal contribution to the gluon effective action. This nonlocality has an unpleasant effect in lattice calculations as it slows down present numerical algorithms dramatically when the quark-masses get small.

In order to elude this problem most numerical simulations in the past have been done in the "quenched approximation" where the determinant is simply replaced by one [1]. More recently, simulations in the "partially quenched approximation" have become available[2], where the determinant gets evaluated at quark masses which are higher than those in the propagators. Thus (partial) quenching amounts to suppressing the contribution of all internal fermion loops in QCD by giving the quarks unphenomenologically high or infinite masses.

Attempts to introduce the corresponding modifications in the low-energy theory artificially in order to learn how to correct for them – the results being "quenched" and "partially quenched Chiral Perturbation Theory" – have shown that the (partially) quenched approximation is, in some aspects, fundamentally different from the full theory: First of all, numerical results won in quenched or partially quenched simulations should (at least in principle) be corrected for the occurrence of "enhanced chiral logarithms" [3,4]. In addition, the η' was found to be a pseudo-Goldstone boson in quenched QCD (as opposed to the situation in QCD, where it is heavier than the lowest-lying octet of pseudo-scalar pseudo-Goldstone mesons by more than a factor $\sqrt{3}$) and its propagator shows – in case the low-energy analysis is correct – a pole of order two (which spoils any field-theoretic interpretation) right at the same position in the p^2-plane where its first-order pole is [3,4]. Even without particle-interpretation, quenched QCD is strictly confined to Euclidean space-time; there is no continuation of its Green's functions to Minkowski space-time [5].

Thus it seems legitimate to search for an alternative starting point for approaching full QCD which gets some qualitative aspects of full QCD right from the beginning.

2 What is "topologically unquenched QCD" ?

The aim is to identify a part of the functional determinant which is cheap from the computational point of view but essential from the field-theoretical point of view.

We start from the generating functional of (euclidean) QCD in the form where the fermionic degrees of freedom have been integrated out

$$Z_\theta^{\mathrm{QCD}}[\overline{\eta},\eta] = N \cdot \int DA\, \frac{\det(D\!\!\!\!/\,+M)}{\det(\partial\!\!\!/\,+M)}\; e^{\overline{\eta}(D\!\!\!\!/\,+M)^{-1}\eta}\; e^{-\int \frac{1}{4}GG\, +i\theta\int \frac{g^2}{32\pi^2}G\tilde{G}} \qquad (1)$$

where $D\!\!\!\!/\, = \gamma_\mu(\partial_\mu - igA_\mu)$ is the (euclidean) Dirac operator and $\tilde{G}_{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\sigma\rho}G_{\sigma\rho}$ the dual of the field-strength operator and where the measure DA includes gauge-fixing and Faddeev Popov terms. In (1) a factor which does not depend on the gauge field to be integrated over has been pulled out of the normalizing factor and the convention is that the quark mass matrix M is diagonal and of rank N_f with the CP-violation stemming entirely from θ (if $\theta \neq \pi\mathbf{Z}$); the shorthand-notation to be used here and in subsequent formulas is $\det(D\!\!\!\!/\,+M) = \prod_{i=1}^{N_f}\det(D\!\!\!\!/\,+m_i)$ in the determinant and $\overline{\eta}(D\!\!\!\!/\,+M)^{-1}\eta = \sum_{i=1}^{N_f}\overline{\eta}_{(i)}(D\!\!\!\!/\,+m_i)^{-1}\eta_{(i)}$ in the propagator.

QCD is known to show a topological structure[6]: The $SU(3)$-gauge-field configurations on $\mathbf{R}^4$ with finite action boundary condition or on the torus $\mathbf{T}^4$ fall into inequivalent topological classes (labeled by an index $\nu = g^2/32\pi^2 \cdot \int G\tilde{G}\,dx \in \mathbf{Z}$). In a given sector ν, any two configurations may be continuously deformed into each other but not into any configuration with a different index ν. Due to this topological structure, the integral in (1) may be rewritten as a sum of integrals over the individual sectors $\int DA \to \sum_{\nu\in\mathbf{Z}}\int DA^{(\nu)}$ and the determinant factorizes ($D\!\!\!\!/\, = D\!\!\!\!/\,^{(\nu)}$)

$$\frac{\det(D\!\!\!\!/\,+M)}{\det(\partial\!\!\!/\,+M)} = \frac{\det(D\!\!\!\!/\,^{(\nu)}_{\mathrm{std}}+M)}{\det(\partial\!\!\!/\,+M)} \cdot \frac{\det(D\!\!\!\!/\,^{(\nu)}+M)}{\det(D\!\!\!\!/\,^{(\nu)}_{\mathrm{std}}+M)} \qquad (2)$$

where the first factor depends on ν only and thus may

be pulled out of the integral. In this form it is obvious that quenched QCD actually does two modifications: It sets both determinant factors equal one, whereas partially quenched QCD keeps both of them at the price of using unrealistically high quark masses.

In "topologically unquenched QCD" the first factor in (2) is kept exact (with the same quark mass as in the propagator between $\overline{\eta}, \eta$) and only the second factor is replaced by one [7], i.e. the "theory" is defined through

$$Z^{\mathrm{TU-QCD}}_{\theta,\{A^{(\nu)}_{\mathrm{std}}\}}[\overline{\eta},\eta] = N \cdot \sum_{\nu\in\mathbf{Z}} \frac{\det(\not{D}^{(\nu)}_{\mathrm{std}}+M)}{\det(\not{D}^{(0)}_{\mathrm{std}}+M)}\; e^{i\nu\theta} \cdot \int DA^{(\nu)}\; e^{\overline{\eta}(\not{D}^{(\nu)}+M)^{-1}\eta}\; e^{-\int \frac{1}{4}GG} \,. \quad (3)$$

At this point, the motivation to treat the two determinant factors in (2) on unequal footing is just an economic one: The "topological" factor is universal for all configurations within one class and bears the knowledge about the nontrivial topological structure of QCD. On the other hand, the "continuous" factor in (2) causes a dramatic slowdown in numerical simulations as this part of the determinant (or its change) has to be computed for each configuration individually.

Note that, in contrast to the full-QCD generating functional (1), the "topologically unquenched" truncation (3) does depend on the choice of reference-backgrounds. Later, two alternative strategies of how to choose, in a given sector, the reference-configuration are described and such a choice of strategy, once it is done, is considered part of the definition of the theory. Obviously there is no a-priori evidence that – with any of these two choices – the approximation (3) should be particularly good. Nevertheless, known analytical knowledge about QCD in a finite box seems to indicate that including the "topological" part of the determinant is sufficient to get some basic features of full QCD qualitatively right.

3 How to implement "topologically unquenched QCD" ?

Obviously, for "topologically unquenched QCD" to be practically useful, at least two requirements have to be fulfilled: First, a recipe of how to make a good choice for the reference backgrounds in (3) is needed. Second, the costs in terms of CPU-time for separating the "topological" part of the determinant from the remainder have to be smaller than the costs would be to compute the determinant as a whole. These issues shall be discussed.

3.1 Upgrading a quenched sample

A quenched sample may get modified to be representative in the sense of "topologically unquenched QCD":

1. Use a method you consider both trustworthy and efficient to compute for each configuration its topological index ν.

2. Use the gauge action you trust to compute, in each class, the gauge-action of every configuration as well as the class-average $\bar{S}^{(\nu)}$ and choose the reference-configuration according to one of the following two prescriptions:

   (i) Choose – out of the class ν – the configuration with minimal gauge-action as the representative $A^{(\nu)}_{\mathrm{std}}$.

   (ii) Choose – out of the class ν – the configuration for which the gauge-action is closest to the class-average $\bar{S}^{(\nu)}$ as the representative $A^{(\nu)}_{\mathrm{std}}$.

3. Use the fermion action and the method you consider both trustworthy and efficient to compute the determinants $\det((\not{D}^{(\nu)}_{\mathrm{std}}+M)/((\not{D}^{(0)}_{\mathrm{std}}+M))$.

4. For any higher topological sector either include the corresponding determinant computed in step 3 into the measurement or eliminate the corresponding fraction of configurations from that sector.

A few points need immediate clarification:

The first problem is that on the lattice, the topological structure of the continuum-theory is washed out; simply computing $\nu = g^2/32\pi^2 \cdot \int G\tilde{G}\, dx$ gives a value for ν which is, in general, not an integer. A solution to this problem is so crucial to the overall performance of the "topologically unquenched" approximation that it shall be discussed in a separate subsection.

The second point is that for computing the determinant ratio in step 3 one cannot rely on any method which is tantamount to an expansion in δA, since the two backgrounds are far from each other. The necessary ab-initio computation is achieved e.g. by the eigenvalue method: typically the first few hundred eigenvalues of the Dirac operator on a given background may be determined.

Finally: What's the difference in terms of physics between the two strategies of how to choose the reference-backgrounds in step 2 ? We emphasize that for either choice there is a sound theoretical motivation. Strategy (i) – choose the configuration which minimizes the gauge action – is nothing but the semiclassical ansatz being pushed to account for topology: Within each sector, the determinant is exact for the configuration having least gauge-action, i.e. for the one which, in a semiclassical treatment, gives the dominant contribution of that sector to the path-integral. Strategy (ii) – choose the configuration which, in its gauge-action, is closest to the class-average of that sector – takes into account that the

Monte Carlo simulation as a whole doesn't try to minimize the total action density but rather the free-energy density: The configuration which is most typical in a certain sector is not the one with minimal action but the one which has additional instanton-antiinstanton pairs plus topologically trivial excitations such as to find an optimum between the additional amount of action to be paid and the additional amount of entropy to be gained. It is the very aim of the second strategy to choose in each sector a "most-typical" background (which realizes such an optimum pay-off) as reference-configuration. It should be stressed that even though the two strategies end up selecting reference-backgrounds which look highly different (exceedingly smooth in the first case versus pretty rough in the second case) the final results may still be close to each other – the only thing which matters is the (strategy-intrinsic) determinant ratio computed in step 3.

3.2 Generating a "topologically unquenched" sample

The fact that the "topological" determinant in (3) is a number which depends only on the total topological charge of the actual configuration but not on its other details suggests that one could try to precompute these "topological" determinants on artificially constructed backgrounds prior to running the simulation.

Within the strictly semiclassical strategy which is reflected by choice (i) the reference-backgrounds are gotten in a rather simple way: Place ν copies (for $\nu > 0$) of a single-instanton solution with typical radius (i.e. $\rho \simeq 0.3$fm, cf. [8]) on the lattice and minimize the action with respect to variation of their relative orientations and positions. Within the more realistic strategy of choice (ii) which accounts for the competing effects of increased action versus increased entropy the reference-backgrounds are constructed as follows: Place ν instantons (for $\nu > 0$) with typical sizes (i.e. $\rho \simeq 0.3$fm, cf. [8]) randomly on the lattice plus additional instanton-antiinstanton pairs such as to achieve a total instanton density of 1fm^{-4} (cf. [8]). Optionally, this background may be dressed with thermal fluctuations by applying a reasonable number of heating-steps (monitoring ν in order to guarantee that it stays unchanged).

Having defined the standard backgrounds in this way a pure Metropolis algorithm generating a "topologically unquenched" sample employs the following steps:

1. Make use of an updating procedure to propose a new configuration and determine its topological index (via the method you trust).

2. If the configuration realizes a previously unseen ν: Evaluate the functional determinant on the standard background constructed for that ν according to your choice of strategy.

3. Base the decision on whether to accept the proposed configuration on

$$\Delta S = S^{(\nu)}_{\text{new}} - S^{(\nu)}_{\text{old}} - \log\Big(\frac{\det(D\!\!\!/^{(\nu,\text{new})}_{\text{std}} + M)}{\det(D\!\!\!/^{(\nu,\text{ old })}_{\text{std}} + M)}\Big) \quad (4)$$

   where $S^{(\nu)}_{\text{new/old}}$ denotes the gluonic action of the newly proposed / last accepted configuration.

There is one conceptual deficit this algorithm suffers from: The procedure for constructing the standard-backgrounds makes use of knowledge about the size-distribution and partly about the density of (anti-) instantons which was won in previous lattice-studies. In other words: The "topologically unquenched" simulation as outlined above is not entirely from first principles. Moreover, the quality of the final sample depends on how appropriate the artificial backgrounds are which were used in the computation of the standard determinants. Constructing these reference backgrounds is particularly demanding within strategy (ii) as it means that one has to do an a-priori guess which configuration, within a given sector, is "most-typical" in the sense of full QCD. Even if "most typical" is translated into a technical criterion (e.g. the configuration which, in its total effective action is closest to the corresponding class-average of a finite full-QCD sample) there is no other algorithmic solution to this problem than by doing a full-QCD simulation. Thus it is reasonable to construct the reference backgrounds as indicated above, thereby making use of existing knowledge concerning size-distribution and density of instantons in QCD – in particular as there is, for strategy (ii), a final check concerning the quality of the artificial backgrounds: In case the guess would have been just perfect, the a-priori ratios of determinants evaluated on these backgrounds (i.e. the ratios which got used in the "topologically unquenched" simulation) would perfectly agree with the analogous a-posteriori determinant ratios evaluated on the "most-typical" configurations as produced by the run. Accordingly, a procedure one might think of trying in case the agreement turns out to be less than satisfactory is just to start over with the simulation – but this time using the "most-typical" configurations found in the first run rather than the artificial guesses.

3.3 Measuring topological indies

Determining the topological index of a newly proposed background in a way which is fast and reliable is so crucial to the overall-performance of "topologically unquenched QCD" as to justify few remarks about this point.

There are several methods [9] to determine, for a given configuration, its topological index ν. Some of them were recently compared and found to give – when implemented

with sufficient care – to comparable results for the topological susceptibility [10]. Nevertheless, it is clear that in the present case, where nothing is known about the spectrum of the Dirac operator on the background at hand, the field-theoretic method is likely to determine ν in the quickest possible way. However, the fact that on the lattice the relevant operator undergoes thermal renormalization provides a challenge: Simply integrating the Chern density, i.e. computing $g^2/(32\pi^2)\int G^a_{\mu\nu}\tilde{G}^a_{\mu\nu}\ dx$ gives a value which is, in general, not close to an integer; in fact, a histogram-plot over many configurations tends to reveal accumulations near regularly displaced, non-integer values, e.g. near $0, \pm 0.7, \pm 1.4$ etc. There are two options of how to deal with this situation:

The first, simplistic, approach is just to define a "confidence interval" – e.g. ± 0.2 – around each of the values $0, \pm 0.7, \pm 1.4, \ldots$ and to assign the configurations lying within these bounds the indices $\nu = 0, \pm 1, \pm 2 \ldots$ etc. The remaining configurations which didn't get an index assigned are then simply tossed away.

The second, more sophisticated, approach is to make use of the fact that cooling a configuration is able to remove the effect brought in by thermal renormalization: Cooling a set of gluon-configurations results in the peaks (in the histogram plot) being shifted closer to the corresponding integers and the valleys between the peaks getting thinned out under each sweep.

The problem is that these two methods do not necessarily agree in their results for a given configuration – a fact which can be understood on rather simple grounds: Under repeated cooling with the naive (Wilson) action, a single-instanton solution shrinks monotonically until it finally falls through the grid. In order to prevent the cooling algorithm at least from loosing the large instantons one has to modify the action w.r.t. which cooling is done in such a way that all instantons with a radius ρ above a certain ρ_{thr} tend to get blown up ("over-improved action") or stay constant ("perfect action") under a sweep, where typically $\rho_{\mathrm{thr}} \simeq 2.3a$. From the evidence given in [11] how quickly cooling with an "over-improved" action tends to pin down $g^2/(32\pi^2)\int G^a_{\mu\nu}\tilde{G}^a_{\mu\nu}\ dx$ near an integer (say 5 sweeps to be within 2.99 and 3.01, etc.) performing $O(3)$ "over-improved" cooling sweeps seems to be sufficient to get an unambiguous assignment. The price to pay, however, is that the small instantons ($\rho < \rho_{\mathrm{thr}}$) get compressed and finally pushed through the grid even more efficiently than under cooling with an unimproved action [11]. From these consideration we conclude that the field-theoretic method with cooling yields, once it has stabilized, a correct assignment for the latter cooled configuration which, however, isn't necessarily appropriate for the initial configuration which may have contained small ($\rho < 2.3a$) instantons. On the other hand, determining the topological index by the first (simplistic) approach (no cooling being involved) has an inferior signal-to-noise ratio (about half of the configurations can't get assigned an index and have to be tossed away) but for the remaining ones the procedure is sensitive to all instantons the lattice can support (i.e. $\rho > 0.7a$).

3.4 Rudimentary cost analysis

The overhead as compared to a quenched simulation results from the CPU-time spent on determining ν for every newly proposed configuration and from the determinants which get evaluated. Preparing the reference-backgrounds and computing the determinants is a fixed investment which is given by L, a, m only (i.e. independent of the length of the simulation) and evaluating the $O(10)$ standard determinants (for nowadays typical values of m and L) is pretty cheap [7]. On the other hand, determining for each configuration its index ν gives rise to costs which grow linearly in simulation-time and thus provide the main overhead (as compared to Q-QCD) in a long run. As a consequence, the method for determining the topological index will have the greatest impact on the overall-performance in TU-QCD. We have advocated choosing a field-theoretical definition with little or no cooling at all, which means that either $O(3)$ cooling-sweeps are performed or 50% of the configurations have to be tossed away. Accordingly, in an approximation where a cooling-sweep is considered twice as expensive as a complete update, the overhead from ν-determinations is roughly a factor 2...6 over a quenched simulation. Thus doing a "topologically unquenched" run might be considered an alternative to a high-statistics quenched run.

4 What about qualitative features of "topologically unquenched QCD" ?

In "topologically unquenched QCD" a determinant is introduced which – as is seen from (4) – only influences the relative weight of the different topological sectors; within each sector there is no difference to quenched QCD.

For QCD in a finite box Leutwyler and Smilga have shown that in the regime [a] $V\Sigma m \gg 1$ the distribution of topological indices is gaussian with width [12]

$$\langle \nu^2 \rangle = V\Sigma m / N_f \quad . \tag{5}$$

In quenched QCD the corresponding distribution is much broader as there is no determinant which suppresses the higher sectors. In "topologically unquenched QCD" the standard determinants result in the higher sectors being suppressed as compared to a quenched sample but the

[a] $\Sigma = \lim_{m\to 0}\lim_{V\to\infty}|\langle\overline{\psi}\psi\rangle|$, where $m_i = m\ \forall i$ for simplicity; note that $V\Sigma m \to \infty$ when $m \to 0$ as the box has to be scaled accordingly: $L \simeq 1/M_\pi, M_\pi^2 \simeq \Lambda_{\mathrm{had}} m$.

amount of suppression strongly depends on the strategy for selecting or constructing the reference backgrounds.

In strategy (i) a sectorial determinant is introduced which is exact for the background which – from the classical point of view – dominates that sector. The point is that this semiclassical treatment is indeed justified for sufficiently small coupling-constant, i.e. in a ridiculously small box where the topological distribution in QCD is known to be extremely narrow [12]. As the box-volume increases the effective coupling gets stronger and strategy (i) is unable to account for this change. To see this more clearly we stipulate the validity of the index theorem on the lattice [9] which allows us to rewrite the two factors in (2) using the Vafa-Witten representation [13]

$$\frac{\det(D\!\!\!\!/^{(\nu)}_{\rm std}\!+\!M)}{\det(D\!\!\!\!/^{(0)}_{\rm std}\!+\!M)}=\prod_{i=1}^{N_f} m_i^{|\nu|}\cdot\frac{\prod_{\lambda>0}({\lambda^{(\nu)}_{\rm std}}^2+m_i^2)}{\prod_{\lambda>0}({\lambda^{(0)}_{\rm std}}^2+m_i^2)} \quad (6)$$

$$\frac{\det(D\!\!\!\!/^{(\nu)}\!+\!M)}{\det(D\!\!\!\!/^{(\nu)}_{\rm std}\!+\!M)}=\prod_{i=1}^{N_f}\frac{\prod_{\lambda>0}(\lambda^{(\nu)\,2}+m_i^2)}{\prod_{\lambda>0}({\lambda^{(\nu)}_{\rm std}}^2+m_i^2)}\quad . \quad (7)$$

Strategy (i) retains a determinant which is appropriate in a small volume and thus strongly suppresses the higher topological sectors. As it comes to larger volumes, the semiclassical treatment breaks down and the quantum fluctuations packed into the "continuous" determinant (7) prove able to milder the suppression – in full QCD, but not within strategy (i). The virtue of strategy (ii) is that this change is accounted for by successively redefining the standard-backgrounds used in (6). In other words: Within strategy (ii) parts which would belong to (7) in (i) are gradually reshuffled into the "topological" part (6) as the box-volume increases. As a consequence, either strategy is supposed to be trustworthy as long as $V\Sigma m \leq 1$, but only strategy (ii) may give a reasonable approximation to full QCD in the regime $V\Sigma m \gg 1$.

Comparing the two factors (6) and (7) one ends up realizing that the "topological" determinant (6) has exactly the same structure as its QCD counterpart (the latter comes without the subscript "std" in the numerator): The essential ingredient is the prefactor $m^{|\nu|}$. In QCD, this prefactor is known [12] to cause the strong suppression of nonzero indices in the limit $V\Sigma m \ll 1$. The fact that it is still around in the "topologically unquenched" approximation (with either choice for the reference-backgrounds) means that TU-QCD (unlike Q-QCD) shows the phenomenon of chiral symmetry restoration if the chiral limit is performed in a finite box.

Finally, the fact that the number of virtual quark-loops is not restricted in TU-QCD means that there is an infinite number of diagrams contributing to the η'-propagator (not just the connected and the hairpin diagram as in Q-QCD) and this propagator may even be well-defined in the field-theoretic sense.

In summary, the fermions in "topologically unquenched QCD" are fully dynamical, but they interact in a way which does not pay attention to the details of the gluon background configuration but to its topological index only and this seems to be sufficient to get a number of basic features of full QCD qualitatively right.

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